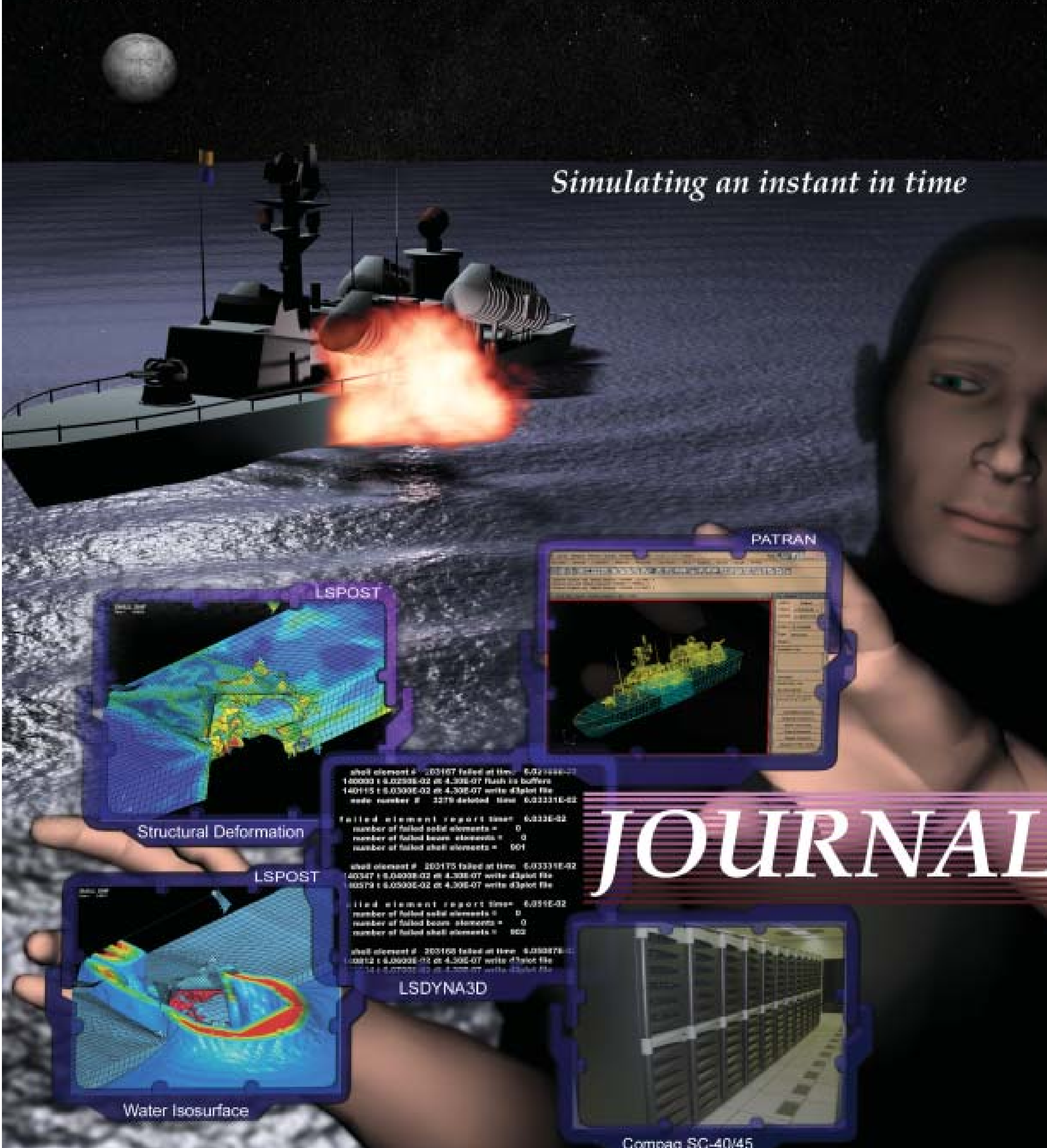
SPRING 2003

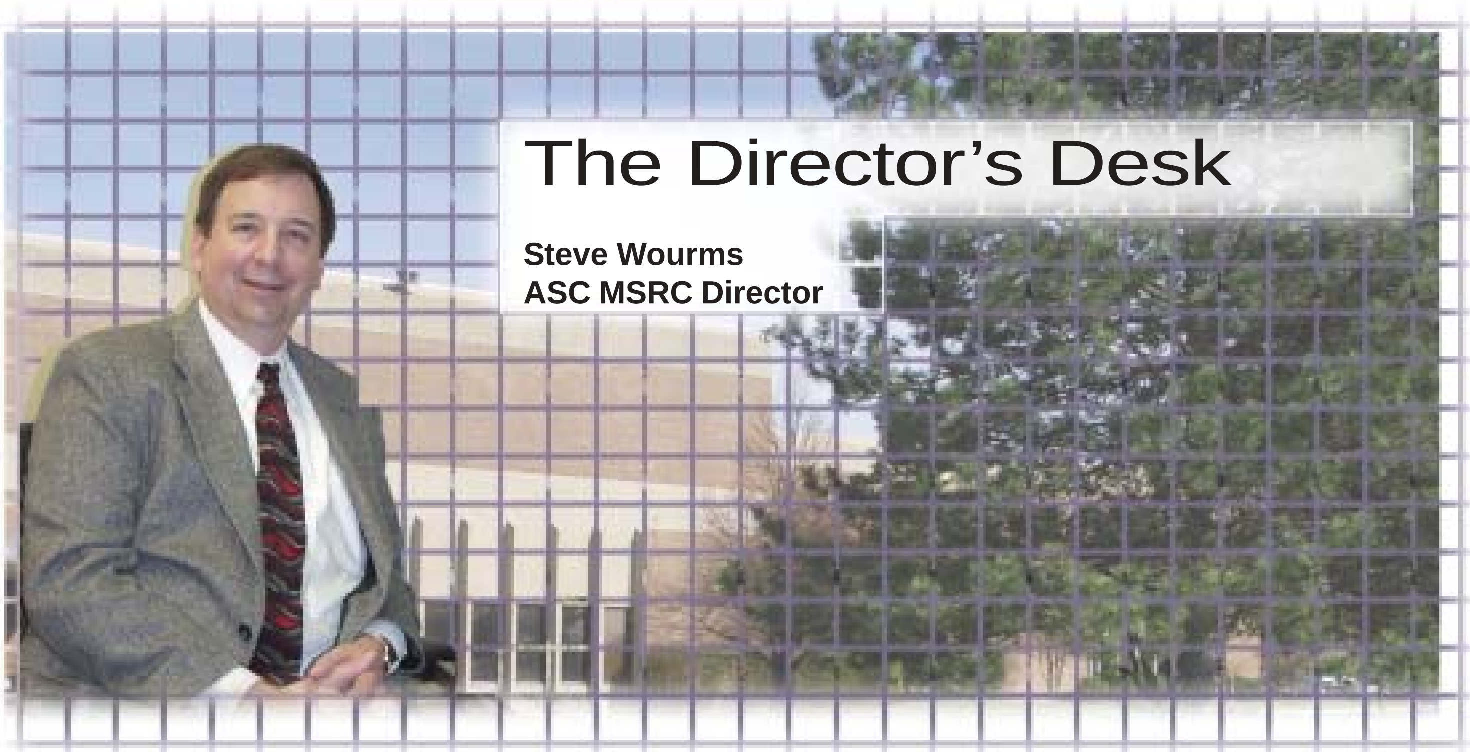
ASC MSRC

AERONAUTICAL SYSTEMS CENTER MAJOR SHARED RESOURCE CENTER

Simulating an instant in time

JOURNAL





The Director's Desk

Steve Wourms
ASC MSRC Director

Silly me. I figured that calendar year 2003 would bring a slower pace to the shop; a chance to get caught up with all those nigglin' little chores that have piled up. Some time to clean out the E-mail folders; sort through the mounds of reports, papers, etc.

Yeah, right.

A huge SGI system will be added as the result of TI-03. We're transitioning to a new support contract. We need to get Instrumental, Inc. cookin'. We're also reorganizing our ASC/HPT bunch. Government folks that we have long relied on are being yanked out from under us.

I'm thankful to have the best support staff, Government and contractor, in the Program! They've bailed me out more than once!

You'll find some amazing accomplishments in this edition of our Journal. The projects undertaken this past year by our PET on-sites are truly remarkable, from Dr. Hinrichsen's shockwave project to toolkit developments to a joint multi-disciplinary forum. We're also quite excited about recent additions to our PET on-site staff.

Look over the articles on our hardware additions. We're thrilled to be installing one of the largest SGI Origin 3900 systems in the world; the user community will love it! Also, we're proud to have implemented our Disaster Recovery system, through which a copy of all of our critical data will be maintained at a site far remote from Wright-Patt.

We continue to populate and maintain an extensive library of software applications. Our Computational Technology Center staff stands ready to assist with these HPC software applications. Give them a call!

Finally, we're re-emphasizing our commitment to the user community. Steve Wilson's *Highlight* article explains the depth of the maintenance upgrade completed in October 2002. Extensive steps were taken to minimize downtime and negative impact to our users. Also, please check out our article on how we ensure our users receive top-notch Customer Support here at the ASC.

My staff and I look forward to your observations and suggestions. Let us know how we can better serve you.

About the cover
The cover illustrates the capability of HPC software and hardware to recreate an instant in time. By manipulating these tools, the user is able to study the extreme forces created by explosions and their affect on war-craft. Data collected can be utilized by all DoD agencies in the continuing effort to improve materials and systems, to better support the warfighter.

The Aeronautical Systems Center (ASC) Major Shared Resource Center (MSRC) is a computational science facility supporting Department of Defense (DoD) research, development, and test and evaluation communities with high performance computing and visualization resources. Created as part of the DoD's High Performance Computing Modernization Program (HPCMP), the ASC MSRC High Performance Computing Center is located on Wright-Patterson Air Force Base (WPAFB) and is one of four DoD MSRC sites. Computer Sciences Corporation (CSC) is the prime support contractor at the ASC MSRC.

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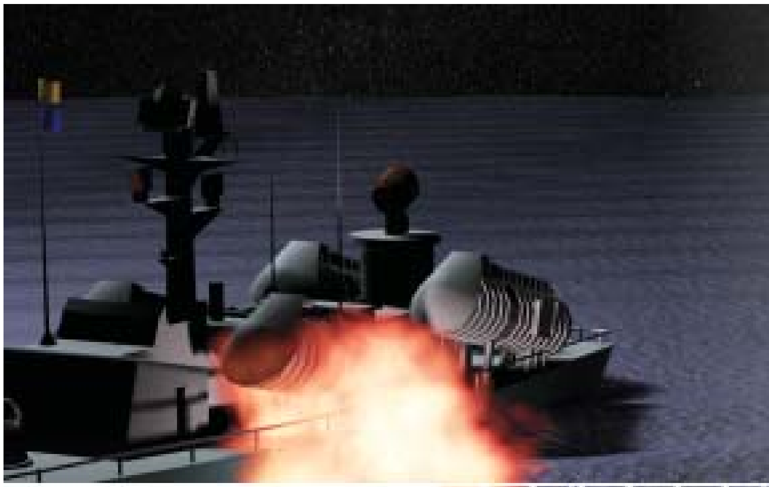
Correction: In the Fall 2002 ASC MSRC Journal there was an error on page 19. The last sentence, in the second paragraph, should have read "What makes QCL operation unique is that as electrons cascade down the conduction band from one stage to another in an almost staircase-like arrangement, photons are emitted." We apologize for any confusion this error may have caused.

Feature

Simulating an Instant in Time

By Ronald L. Hinrichsen



The ASC MSRC provides modeling and simulation (M&S) support to a number of organizations interested in weapon system survivability. This support ranges from providing mentoring and training services for engineers and researchers in the survivability community, to actually performing M&S work on specific weapon and threat systems.

In order to accurately predict how a structure will react to a threat, state of the art software is needed which captures the physics of the encounter. Generally, this means that a coupled Computational Structural Mechanics (CSM)/Computational Fluid Dynamics (CFD) technique must be used. There are CSM/CFD software packages currently used, which capture the necessary physics to simulate these events. In this article, we highlight the capabilities of the LSDYNA3D® code in simulating the detonation of a high explosive charge in close proximity to a surface ship.

In simulating the instant in time when the explosion takes place, the water, explosive charge and air are modeled in a multi-material Eulerian domain. This domain is typical of CFD analysis methods where the mesh is fixed in space and the materials are allowed to flow through the mesh. The structural members of the shell elements, while the blue mesh is the Eulerian ship are modeled in the Lagrangian domain. This domain is typical of CSM analysis methods where the mesh is allowed to deform and move. The Eulerian and Lagrangian domains are loosely coupled together and information (such as position, pressure, etc.) is exchanged at the interfaces of the two domains.

Figure 1 shows two views of the model meshes, which were used for this simulation. The white mesh is the Lagrangian domain, which consisted of shell elements, while the blue mesh is the Eulerian domain, which consisted of brick elements.

One of the capabilities that was effectively used in this simulation was the assignment of the multi-materials to the Eulerian domain. The feature that was used is called *INITIAL_VOLUME_FRACTURE_GEOMETRY. With this feature, the interfaces between water, air, and explosive were defined by specifying air above a given coordinate plane, air within the ship's hull,

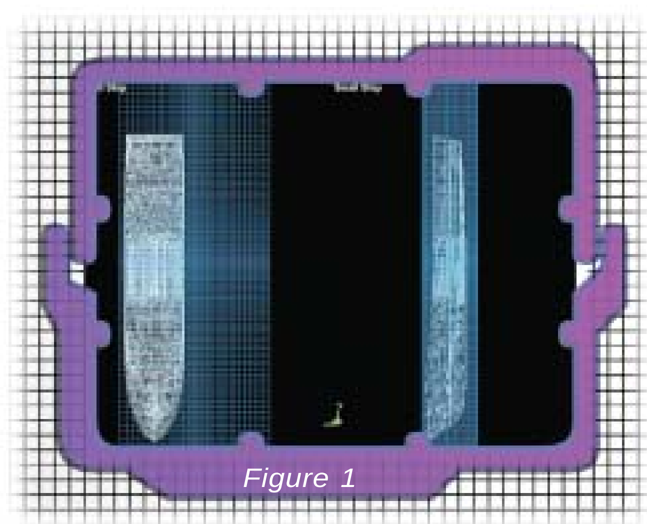


Figure 1

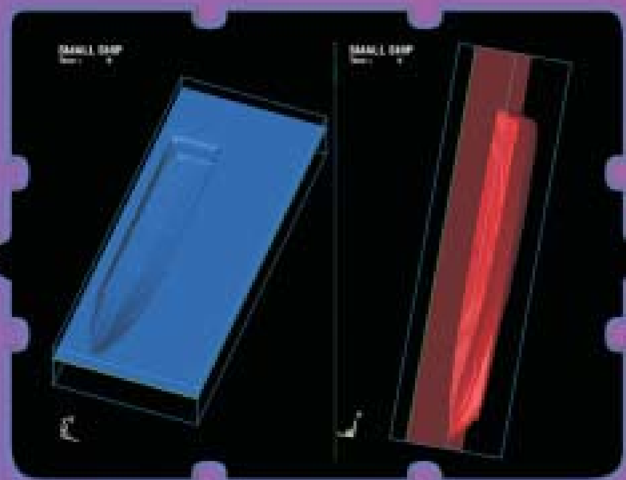


Figure 2

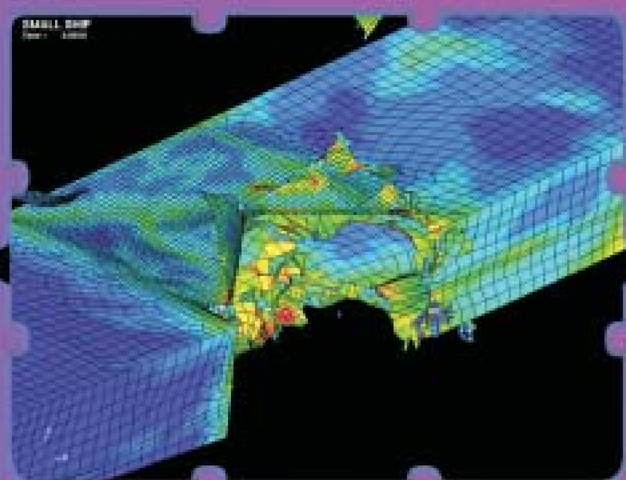


Figure 3

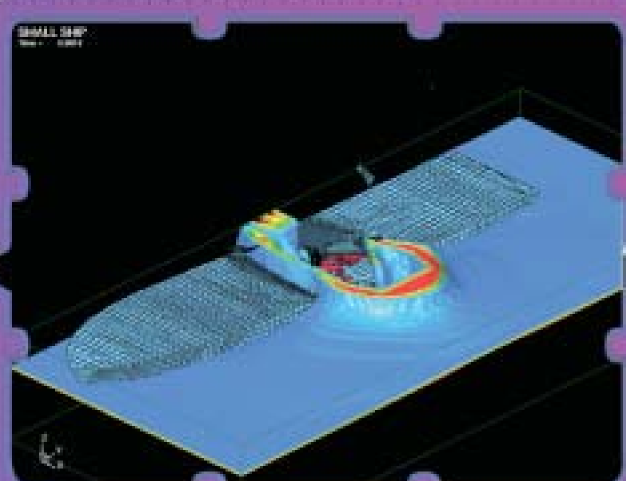


Figure 4

explosive in a sphere located near the ship's hull, and water everywhere else. Figure 2 shows isosurfaces in two views of the Eulerian domain. Everything above the blue isosurface is air. The material is shown in red and below is water and the spherical explosive charge.

At the beginning of the simulation, the spherical explosive was detonated. The high-pressure pulse quickly impacted on the ship's hull, and the hull material failed progressively due to the exceedance of the allowable plastic strain limit.

Figure 3 shows a close-up of the ship's hull with color stress contours superimposed on the model. Figure 4 shows a close-up of the water isosurface showing the water entering the ship through the breech in the hull and overflowing the hull surface as the event occurs.

The simulation of this instant in time (actually 81 milliseconds) was performed using four processors on the Compaq SC-40/45 computers at the ASC MSRC. It required 543 hours of CPU time and ran to completion in 191 wall-clock hours.

M&S of these types of events is valuable in predicting event-outcomes in advance as well as assisting in test planning. If you are interested in this type of M&S, contact Dr. Ronald L. Hinrichsen at *hinricrl@asc.hpc.mil*.

TI-03 Hardware Additions

By Dave Potts and Jeff Graham

The third year of the High Performance Computing Modernization Program (HPCMP) Technology Insertion (TI-03) process has brought exciting new capability to the ASC MSRC. Silicon Graphics, Inc. (SGI) was selected to install the world's most powerful Origin-3000 cluster at the center. The system consists of four 512-processor, 512-GByte Origin 3900s, a 12-processor Origin 3800 front-end, and 40-TBytes of shared workspace disk. These 2048 700-MHz R14000 MIPS processors utilize the IRIX operating system with their batch queues under the control of LSF from Platform Computing. The software support environment includes SGI compilers, SGI debuggers, and several third-party software analysis tools. Additionally, two 64-processor Origin 3900s were installed for classified research, replacing one 64-processor Origin 2000, which has less than one-third of the performance per processor.

The selection of these computers was a lengthy process involving several teams. Representatives from the HPCMO and all MSRCs participated on Benchmarking, Confidence, and Usability teams under the overarching Collective Acquisition Team (CAT). The Benchmark team began its work in May 2002. Based on previous years' work, a benchmark package was organized and released to potential vendors during July 2002. The CAT began its work in early 2002 and released a Request for Quotes (RFQ) to participating vendors in August 2002. The Confidence and Usability Teams began their work during June 2002. The initial evaluation of vendor submitted data was accomplished during the first half of October. In November 2002, vendors were asked for Best-and-Final Pricing for the most promising configurations. During the December CAT meeting, the final solutions were selected. General Services Administration (GSA) negotiated the final contracting details and announced the selections during January 2003.

The ASC MSRC team began work during April 2002, in preparation for the TI-03 process. Knowing that the ASC MSRC was targeted for a major upgrade, Mr. Steve Wourms, ASC MSRC Director, challenged the in-house team to make a "big splash" for our users, our MSRC, and the HPCMP. This in-house team reviewed the current and past ASC experiences and strategies for optimum HPC environments. Past utilization data and the current program requirements survey were reviewed. Programming Environment and Training (PET) leads were interviewed on the issue of "work flow", which was of special interest in sizing potential HPC solutions. The facility's capacity at ASC was also analyzed. All these factors were incorporated with the potential scenarios of HPC equipment for ASC.

At the ASC MSRC we are thrilled to have made such a "big splash", which will supply HPCMP users with nearly eighteen million CPU-hours per year of the fastest IRIX machines available. All four 512 processor systems should be finished with Effectiveness Level Testing (ELT) by the end of June 2003. FY03 allocations (totaling over 3 million hours) should be available beginning 1 July 2003. Due to a staggered delivery schedule, it is anticipated that a total of 1024 processors will be available as early as 1 July 2003, with the remaining 1024 processors available 1 August 2003. Initial comments from users indicate that these systems will be heavily utilized right from the start.

ASC is delighted that SGI systems are available along with the Compaq SC-40/45 and the IBM P3 for our HPCMP users. For the most up to date information visit our website at *www.asc.hpc.mil* or contact the MSRC Service Center at *msrchelp@asc.hpc.mil* or 1-888-677-2272.

Disaster Recovery at the ASC MSRC

By Vaughn Noga

"The ASC MSRC and the Space and Naval Warfare Systems Center – San Diego (SSC-SD) have entered into a partnership to provide mutual disaster recovery capabilities."

– Lisa Burns 'The New ASC MSRC Disaster Recovery System'

Prior to the events of September 11th, 2001 we realized a deficiency existed with respect to the ASC MSRC's ability to protect users' data. How sobering it was to witness how vulnerable we really were. Within days of the "9/11" tragedy we began actively investigating methods by which we could assure our users' data was protected in the event of a local catastrophe.

As we began our investigation we kept three criteria central to how we would implement our system:

- Leverage the Defense Research and Engineering Network (DREN) to facilitate and protect the wide-area dissemination of our data to a remote facility.
- Leverage existing HPCMP software procurements (SUN SAM-FS) to provide a global HPCMP model that other centers could follow.
- Eliminate the need for special equipment to recover our users' data to other MSRCs.

The better part of a year was spent evaluating various Disaster Recovery (DR) sites, architecting the solution, and planning for the eventual integration effort. In December 2002 a team of highly skilled and motivated individuals journeyed 2,300 miles to SSC-SD to begin the weeklong integration. ASC MSRC personnel Ralph McEldowney, Vaughn Noga, Tracey Wilson, and Bobby Nutting (SSC-SD) spent many long hours installing and configuring the network, storage, and ancillary systems.

"How sobering it was to witness how vulnerable we really were."

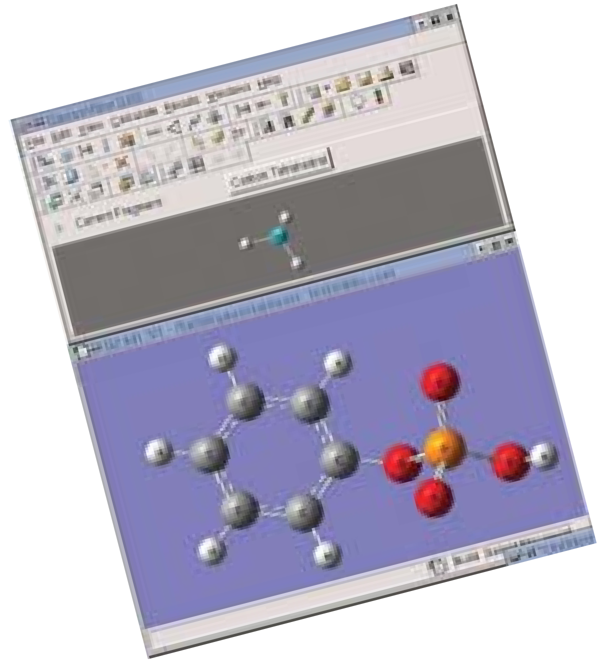
Within days of our arrival we had stood up the encrypted network, verified connectivity, and integrated all the storage/ancillary servers. By the end of the week we were able to successfully demonstrate the migration of files from the ASC MSRC to the SSC-SD, and the subsequent restoration of those files back to the ASC MSRC. The systems entered into Effectiveness Level Testing (ELT) on December 18, and successfully passed the 30-day ELT and Capabilities Test. The systems were placed into production on January 18, 2003.

Functionally, the new DR system performed magnificently. We were able to migrate data from our local system to the remote system with little to no intervention. However, we did encounter one issue as we went into production – *transfer rate*. We soon began to realize that our wide-area SAM-FS transfer rate was surprisingly low. After some local troubleshooting we concluded that there was something awry with how SUN's SAM-FS transferred data over the WAN. Working directly with the SUN/LSC developers, we discovered problems with how data migration was managed through SUN's SAM-ftpd process. After much direct communication and new code development, we were able to obtain transfer rates 10X over our initial transfers. We now have a system capable of migrating hundreds of gigabytes of data per day.

At the time of this writing we have successfully transferred the most recent 150 days of users' data ~ 5 TB and ~ 5TB of backup data and logs. By early summer, we expect to have migrated 30% of our archive – roughly 20TB.

Additions Made to the ASC MSRC Software Baseline

By Casey Doty



Several HPC software applications have recently been added to the ASC MSRC baseline as a result of the Technology Insertion (TI-03) process. These additions reflect the continuous effort of the ASC MSRC to meet our users' needs.

ANSYS - Pro/Engineer (Pro/E) Connection

The Pro/E connection module for the Computational Structural Mechanics (CSM) product ANSYS will allow users to move data quickly and cleanly between ANSYS and Pro/E. This product imports actual geometry from the supported CAD system, without parameters or associativity, increasing the user's productivity while lowering time usually spent for geometry cleanup.

GaussView

GaussView is a full-featured graphical user interface (GUI) for Gaussian 98. With GaussView you can construct molecular systems of interest using its molecule building facility. GaussView allows the setup, execution, monitoring, and post-execution examination of Gaussian calculations.

Gaussian is one of the most utilized Computational Chemistry and Materials Science (CCM) codes at the ASC MSRC. With the addition of this GUI, Gaussian users will find it much more convenient and attractive for them to do research with Gaussian.

Jaguar (Parallel)

Jaguar was designed to increase the speed of ab initio calculations in order to accelerate basic and applied research projects and to enable calculations at a higher level of theory. Jaguar provides the ability to study many systems, within a reasonable timeframe. Currently, a serial version of Jaguar is installed on all HPC platforms at the ASC MSRC. The addition of the parallel version of Jaguar will enable more CCM users to run calculations on our HPC systems.

STAR-CD (Chemkin Module)

STAR-CD/KINetics combines the Computational Fluid Dynamics (CFD) and geometry-handling strengths of STAR-CD with components of CHEMKIN's leading-edge technology for treating complex coupled chemical kinetics and molecular transport. This module provides superior reaction modeling capabilities compared to standard equilibrium chemistry models that are standard in STAR-CD or Fluent. The improved Kinetics modeling provided by STARCD/KINetics is essential for accurate simulation of combustion dynamics for state-of-the-art propulsion systems.

Gaussian03

In addition to these new applications, an update to Gaussian has been installed on the HPC platforms. Gaussian03 is the newest version of the Gaussian program, which is a popular quantum mechanics package widely used by the CCM user community.

This new version of Gaussian provides a wide variety of new and enhanced modeling capabilities that increase both the range of chemical problems and the size of molecular systems that can be studied. The Polarizable Continuum Model (PCM) solver has been improved and extended, and molecular dynamics calculations are available in Gaussian 03. Many new molecular properties such as spin-spin coupling constant, g tensors and other hyperfine spectra tensors, harmonic vibration-rotation coupling, anharmonic vibration and vibration-rotation coupling are also provided in Gaussian03.

Additional information can be obtained by contacting the ASC MSRC Service Center at 1-888-677-2272 or via email at *msrchelp@asc.hpc.mil*. ASC MSRC users may view a list of currently available software on our website.

MSRC Transitions to New DREN Service

By Ralph McEldowney

The ASC MSRC transitioned to a new Defense Research and Engineering Network (DREN) service in January 2003. DREN provides wide area networking connectivity between DoD HPC centers, HPC users, and the Internet.

Between July 1997 and January 2003, AT&T provided DREN service at the MSRC. The initial capability in 1997 was an IP-only service over an Asynchronous Transfer Mode (ATM) OC-3 uplink circuit. Multiple upgrades in subsequent years increased the capabilities to include ATM service and increased the uplink circuit to ATM OC-12. The AT&T DREN backbone was based on ATM technology, supporting both native ATM and IP-over-ATM services on the same network.

In January 2003, DREN service transitioned from AT&T to WorldCom. Like AT&T, the WorldCom service includes both IP and ATM services; however, the WorldCom DREN backbone is based on Packet Over SONET (POS) technology and uses Multi-Protocol Label Switching (MPLS) to maintain logical separation between the IP and ATM services. IP service may be delivered over Fast Ethernet, Gigabit Ethernet, or 10 Gigabit Ethernet interfaces, while ATM service may be delivered over OC-3 or OC-12 ATM interfaces. Uplink circuits, which connect the DREN site to the backbone, may be configured as DS-3, OC-3, OC-12, OC-48, or OC-192 POS connections.

Network Bandwidth in million (M) or billion (G) bits per second (bps).

Ethernet	10 Mbps
DS-3	45 Mbps
Fast Ethernet	100 Mbps
OC-3	155 Mbps
OC-12	622 Mbps
Gigabit Ethernet	1 Gbps
OC-48	2.5 Gbps
10 Gigabit Ethernet	10 Gbps
OC-192	10 Gbps
OC-768	40 Gbps

The ASC MSRC receives both IP and ATM services from WorldCom. The IP service is delivered over a Gigabit Ethernet interface, while the ATM service is delivered over an ATM OC-12 interface. The uplink circuit into the backbone is an OC-12 POS circuit.

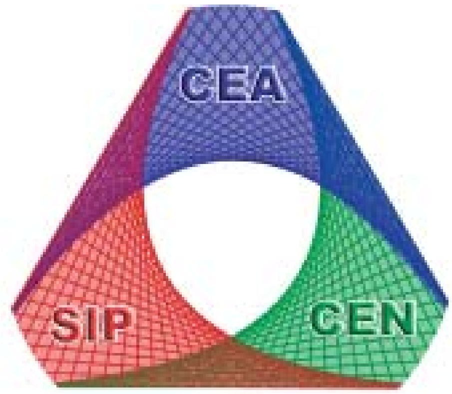
All 80 DREN sites receive services through individual Service Delivery Points (SDP). The SDP consists of equipment owned, operated, and maintained by the provider. In other words, the government buys a service, not a network. The advantages of this model include the ability of the government to leverage the expertise, experiences, and best practices of industry.

WorldCom must meet very strict DREN Service Level Agreements (SLAs) including latency, IP packet loss, ATM cell loss, and throughput parameters. Regarding throughput for example, WorldCom must guarantee that every SDP can sustain 50% of the uplink bandwidth at any time, and burst to 80% of the uplink bandwidth for tens of minutes. In addition, the new DREN network will support several new technologies such as IP version 6 (IPv6) and native Multicast capabilities.

The new DREN service from WorldCom will be very beneficial for the ASC MSRC and its users. High capacity bandwidth, connectivity to other research networks, strict SLAs, and new technologies will benefit the entire MSRC community. For additional information or to report problems with the MSRC network or DREN connectivity, please contact the MSRC Service Center at 1-888-MSRC-ASC.

SIP/CEA/CEN Joint Forum

By John Nehrbass



"Use of High Performance Computing in Interdisciplinary Engineering", the first PET sponsored Signal Image Processing/Computational Electromagnetics and Acoustics/Computational Electronics and Nanoelectronics (SIP/CEA/CEN) Joint Forum, was held November 5, 2002 in College Park, Maryland. This, by-invitation only meeting, provided a forum for participants to express their views on the needs for HPC technology in SIP/CEA/CEN. Included were paper presentations, overviews of current DoD research activities, as well as spirited discussions on future research directions.

HPC trends, such as high-performance scalable parallel processing; computer clusters; relative standardized simulation environments; and Simulation Based Acquisition (SBA) have progressed in the past years. These trends suggested that a forum to review the current state of the art in the application of HPC to SIP/CEA/CEN was warranted. Accordingly, PET co-sponsored a forum focused on the role of HPC in the overlap areas across SIP/CEA/CEN.

For many engineering systems, the ability to perform end-to-end simulations that allow engineers to assess system performance under a variety of possible conditions is highly desired. With the advent of HPC and the development of efficient numerical techniques, the dream of system engineers to perform end-to-end system simulation is becoming a reality. It has become increasingly apparent that there are a number of engineering problems in which these three computational areas, SIP, CEA, and CEN, intersect and that there are significant opportunities to benefit a number of DoD programs. An example of such an engineering problem is the end-to-end assessment of an ad hoc mobile wireless system for which a number of issues, such as efficient amplification, low-power operation, signal processing, waveform generation and modulation, filter – diplexer - and antenna miniaturization, radiation in the presence of complex platforms, wave propagation in a multi-path and highly scattering environment, co-site interference, and many more, must be addressed.

Bringing together a select group of researchers with diverse expertise helped the HPCMP identify areas of critical need for DoD research. This inaugural forum provided the collective community with a unique opportunity to identify critical SIP/CEA/CEN problems that could, and should, be the focus of DoD HPC research and resources. Additionally, this forum provided a venue to describe the on-going activities and services of the Common HPC Software Support Initiative (CHSSI) and PET programs, and solicited guidance from the larger community as these programs continue to support the DoD community in HPC.

Each Government Computational Technology Area (CTA) leader provided a perspective on the issues of HPC in interdisciplinary engineering for their CTA. This was followed up with an overview of activities within the HPCMP presented by all three PET Functional Area POCs (FAPOC). Dr. Barry Perlman, principal investigator for the Electronic Battlefield Environment Portfolio, provided a short overview and showed how discussions around his portfolio are well matched for the forum.

Several key points were identified at the SIP/CEA/CEN Forum. Some of these ideas are presented here:

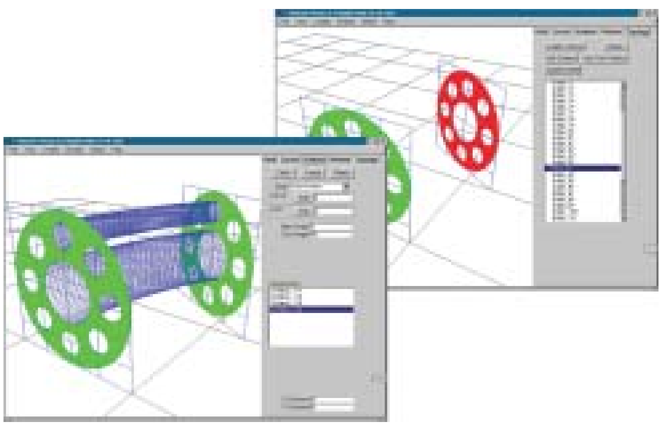
- The SIP community seems to be identified with the DoD operational community, while the CEA community seems to be identified with the DoD acquisition community. The contrast between these two communities may create possible barriers that prevent groups from forming common ground, required for interdisciplinary research.
- To interact effectively, a common language must be identified.

- A good motivation may be solving operationally challenging projects that have a very immediate effect on the warfighter. Simulating the complexity of urban warfare is a good example.
- It was mentioned several times that many SIP problems deal with the temporal solutions of Maxwell equations, while CEA problems deal with the spatial solutions of Maxwell equations. Interesting initial projects could be projects where SIP systems become driven by synthetic data generated from CEA systems.
- A good method for testing and validating cross-CTA complex systems must be developed. A real danger is to start producing wrong answers for the warfighter or promoting false expectations of quick solutions to extremely difficult physics problems.
- A clear definition of what kind of information is required by a SIP system from a CEA system is necessary. The interfaces between the systems have to be unambiguous and specified in a common language.
- An important task is to adopt an architecture that will permit interoperability among systems (XML, HLA, CORBA, etc.) and to start investing in converting the interfaces of existing codes to comply with the architecture. This will require a major resource commitment by the individual CTAs.

A CD-ROM of the proceedings can be obtained, with pending security approval, by contacting any active members of the SIP, CEA, or CEN PET teams, or by contacting the MSRC Service Center at *msrchelp@asc.hpc.mil*.

Geometry-Grid Toolkit

By Hugh Thornburg



For the past two years, the PET Computational Fluid Dynamics (CFD) team, University of Alabama Birmingham (UAB) and Mississippi State University researchers have been working together to develop the Geometry Grid Tool Kit (GGTK). This toolkit builds upon years of successful efforts in the area of grid generation and geometry modeling for computational field simulation. Funding for this effort has been provided by the National Aeronautics and Space Administration (NASA), the National Science Foundation (NSF), and the DoD PET program. The data structure has been designed to allow geometry definition, topology and mesh generation to use a common data structure. A GUI-based system (MiniCAD) is included to exercise the functionalities of GGTK.

GGTK is a comprehensive library containing computer aided geometry design (CAGD) and geometry, topology and mesh generation functionalities accessible from FORTRAN, C, and C++ application programs. Included are capabilities in the area of CFD-based shape optimization, adaptive meshing, and mesh generation templates for automatic and parametric mesh generation suitable for multidisciplinary and moving body problems. GGTK is also being used in the NSF Information Technology Research (ITR) program to demonstrate seamless multidisciplinary analysis (chemically reacting fluid, heat transfer, structures, and fatigue/crack growth) using the parametric description of geometry.

The alpha version of the GGTK along with proper documentation and GUI-based MiniCAD system is available for distribution. Many capabilities of interest to the DoD communities are included. However the package is still undergoing enhancement, development and testing. The developers solicit feedback in terms of additional functionalities desired, possible bugs and ease of use.

DoD users may request the package by contacting Dr. Alan M. Shih of UAB at *ashih@uab.edu*.

PET Technical Review Shares Scientific Goals and Achievements

By Brian Schafer

Members of the HPCMP community gathered at Clark-Atlanta University for the PET Technical Review, February 3-6, 2003. In attendance were the HPCMP Director, center directors, PET program manager and leadership team, and government Computational Technology Area (CTA) leads. Also attending were the MOS and HPTi PET leadership team, Functional Area Points of Contact (FAPOCs), and PET on-sites.

This was the first time since the PET II contract was awarded that the government and contractor leadership team have had the occasion to meet and share thoughts at one location. This afforded the PET contractors the opportunity to share their triumphs and challenges, and discuss how functional areas can succeed together.

PET Component 2 is responsible for PET efforts in four functional areas:

- Forces Modeling and Simulation /C4I (FMS)
- Integrated Modeling and Test Environments (IMT)
- Signal/Image Processing (SIP)
- Enabling Technologies (ET)

Dr. Dave Pratt, FMS FAPOC, is concentrating his resources on reaching out to the DoD FMS community. Because FMS is a non-traditional HPC area, a concerted effort is being made to "create the market" for HPC services and resources and to assist in the transformation of the FMS community's perceptions of HPC. One method of Outreach is to create projects that aid the transition of experience in the HPC community to the FMS community. These projects illustrate how FMS codes can be ported to HPC machines, parallelized, and optimized, greatly improving application runtime. One of the major facilitation mechanisms is the growth and acceptance of scaleable Linux cluster technologies and machines. This provides a means for users to run small simulation exercises locally and come to the MSRC for the "heavy lifting" with minimal, if any, modifications to the software configuration. Dr. Pratt also highlighted Dr. Phil Amburn and the ASC staff support for the exercise with JFCOM. (*See related article page 12.)*

One of the key challenges facing the Test and Evaluation (T&E) community is how to assimilate huge datasets generated by testing activities. PET IMT personnel are endeavoring to develop rules and formats for archiving data for easy retrieval. These capabilities will improve the flow of information between T&E Centers and between the Test Centers and the acquisition communities. Expensive, high fidelity test data can be effectively reused resulting in a faster, and improved, weapon system development process. Results from these efforts are applicable to the other functional areas such as SIP's sensor fusion efforts.

Dr. Tilt Thompkins, IMT FAPOC, also foresees IMT's opportunity to shape software architectures so that test integration through high performance simulation begins early in the development process. As a result, evaluations can account for all available information and test planning can proceed down the most cost effective paths.

The SIP functional area addresses three communities:

- Real-time/Embedded
- Algorithm Develop and Test
- Simulation and Verification

Each community's HPC needs can differ dramatically. The strategy of Dr. Stan Ahalt, the SIP FAPOC, is to serve these three communities by providing training, leadership through Outreach, dissemination, and demonstration, and significant SIP project impacts. One of the most pressing needs in the SIP community is addressing the challenge of exploiting all the information that is present in the myriad of signals harvested from deployed DoD sensors. Extracting and transforming the information is essential if the collected data is to be exploited by our soldiers, officers, security personnel, and senior civilian decision makers. Dr. Ahalt described past, present, and proposed efforts that address long- and short-range surveillance, individual identification, biometrics, voice modification, and sensor webs. SIP is collaborating with other functional areas such as ET and IMT to develop techniques in distributed computing, data mining and understanding, cognitive processing, and embedded computing to support these applications.

ET advances the state of tools, algorithms and standards for pre- and post-processing of very large datasets. This includes, but is not limited to scientific visualization (SciVis), data mining and knowledge discovery, image analysis, grid generation, problem solving environments (PSEs), and computational techniques for intelligent extraction of useful information. ET supports work performed in other computational technology areas.

Dr. Robert Moorhead, the ET FAPOC, recognizes the focus of ET is on HPCMP users as opposed to HPCMP resources. By developing tools such as the HPCMO Computing Portal, ENVis, Geometry-Grid Toolkit (GGTK) (*see related article page 9)*, and the Integrated Simulation Environment, ET is providing the means for DoD users to better explore and understand massive datasets.

Other FAPOCs in PET Components 1, 3, and 4, presented similar briefings describing past accomplishments and future efforts. All fifteen of the FAPOC's presentations are available on the PET Online Knowledge Center at *https://okc.erdc.hpc.mil* under the Papers and Presentations section.

At the conclusion of the PET Technical Review, everyone had a better understanding and appreciation for the breadth and depth of the work performed under PET. Participants came away with a stronger desire for functional areas to work closer together to improve effectiveness, share lessons learned, and provide a greater impact to the DoD.

FMS On-site Lead Named

By Brian Schafer

Dr. Philip Amburn has been named the PET on-site lead for Forces Modeling and Simulation (FMS/C4I) at the ASC MSRC. He is employed by Science Applications International Corporation (SAIC), supporting Dr. Dave Pratt, the PET Functional Area Point of Contact (FAPOC) for FMS.

Dr. Amburn received his Ph.D. in Computer Science from the University of North Carolina in 1994, specializing in interactive 3-D computer graphics and virtual environments. Before joining the PET team, Phil worked both in academia and in private industry.

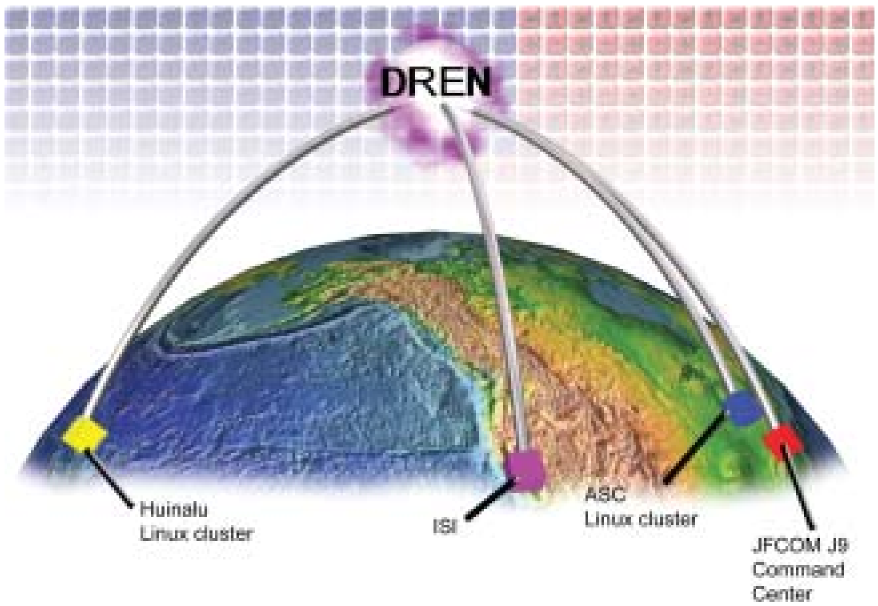
Phil began his career with the Air Force in 1973, joining the Strategic Air Command Headquarters as a computer programmer. By 1987, he was an instructor of Computer Science at the Air Force Institute of Technology. Specializing in computer graphics, Phil became the principal investigator for the Distributed Interactive Simulation project, which included flight simulation and battlefield viewers on Silicon Graphics workstations.

After retiring from the Air Force in 1994, Phil joined SAIC, working in Albuquerque, New Mexico and Dayton, Ohio. As a senior computer scientist, Phil worked on a PC implementation of J-MASS, an Air Force modeling and simulation architecture. He was also involved in the early formation of the Simulation and Analysis Facility (SIMAF).

Next, Phil used his imaging expertise in the medical field when he joined Qualia Computing, Inc. in 1997. He was the product manager for Second Look™ Breast Cancer Computer-Aided Detection. He also prepared grant applications and project descriptions for new product concepts and was involved in evaluating product concepts for Qualia to pursue.

As a PET FMS on-site, Phil is responsible for reaching out to the DoD FMS community through training, transferring innovative HPC technology from academia to the DoD, and facilitating collaborative activities with academia, government and industry. Away from the office, Phil follows the trials and tribulations of the University of North Carolina basketball team. His two favorite teams are UNC and WHOEVER is playing Duke.

JFCOM J9



By Philip Amburn

Joint Experimentation on Scalable Parallel Processors (JESPP) III is the third phase of a long-term multi-phase effort by Joint Forces Command (JFCOM) J9 (Joint Experimentation Directorate). This effort provides very large scale 'wargame' like experiments, involving millions of entities (e.g., planes, tanks, trucks), which represent a rich mixture of current-day and hypothetical capabilities and behaviors. These experiments allow military organizations to explore and evaluate the interactions of alternative equipment, doctrine, training, personnel, environmental, and other factors in settings with a high degree of fidelity and realism. The long-term goals are to:

– Build the infrastructure for the enormous computational demands of very large scale experiments.
– Develop human-in-the-loop capabilities for initiating, monitoring, controlling, and analyzing the experiments.
– Design and demonstrate techniques for programming richer and more sophisticated simulated entities for participation in the experiments.

This third phase will develop new tools to enhance communications between the processors of the scalable parallel processors (SPPs), ensure reliable communication to the operator's consoles, enable better reporting and analysis of both exercise and computer performance, and encourage new research into simulation of human behavior.

JFCOM J9 has determined that there is great value in experimentation conducted at the entity level on high-resolution terrain databases. However, current capabilities in personal computer power, hardware and simulation software do not allow experiments at the scale and fidelity desired. Commercial HPC equipment has been used by J9 in previous experiments. A significant part of JESPP III is incorporating HPCMP HPC resources including two Linux clusters and use of the Defense Research Engineering Network (DREN). For JESPP III, the 16-node Linux cluster at the ASC MSRC and the 256-node Linux cluster at the Maui High Performance Computing Center (MHPCC) ran the Joint Semi-Automated Forces (JSAF) software as a constructive simulation generating "entities" at a variety of locations around the world. Figure 1 shows the "play box" for the March 2003 experiment. Blue Force assets included: B2s, KC-10 tankers, C-17s to haul Patriots, Global Hawk unmanned air vehicle (UAVs), convoy ships, submarines, and Patriot batteries. Red Force assets included F-7s, Mig 29s for Red Air combat air patrol (CAP), and surface to air missile (SAM) sites. Over 200 instantiations of JSAF ran on the compute nodes at ASC and MHPCC. Each of these JSAF executables generated high-level architecture (HLA) messages describing the motion and actions of the entities. Software message routers relayed these messages to workstations at J9 in Norfolk, Virginia and engineers and scientists at Information Sciences Institute (ISI) in Marina del Ray, California.

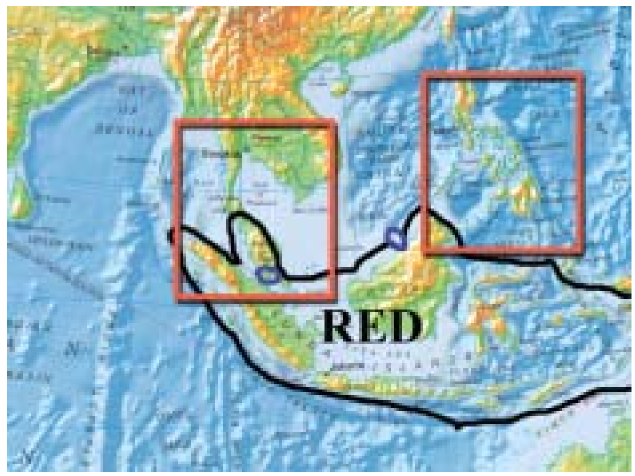


Figure 1. Scenario Map

Operational military personnel at J9 used the Plan View Display (PVD) (see Figure 2) to observe the actions of JSAF controlled entities. When needed, operational personnel issued commands from their terminals and their network messages modified the actions of individual entities or groups of entities. Figure 3 is an example of a 3-D display of a battlefield, often called a “stealth view”.

JESPP III was conducted March 24-28. Dr. Ronald Sega, Director of Defense Research and Engineering, visited JFCOM J9 and observed a portion of JESPP III. He was impressed with the on-going experiment and noted the applicability of the technology to other areas of research in the DoD. This experiment laid the foundation for continued work.

JFCOM’s web site describes J9’s responsibilities, “As the transformation laboratory for the Department of Defense, USJFCOM turns to the Joint Experimentation Directorate (J9) to develop, explore, test, and validate 21st-century warfighting concepts. Joint warfighting transformational concepts developed here will be integrated into future joint forces training. Through the process of experimentation, USJFCOM will ensure that our military force of tomorrow can fight more effectively, more efficiently, and at less risk than in the past. To that end, joint experimentation offers improvements in doctrine, interoperability, and integration, all of which lay the foundation for defense transformation.”

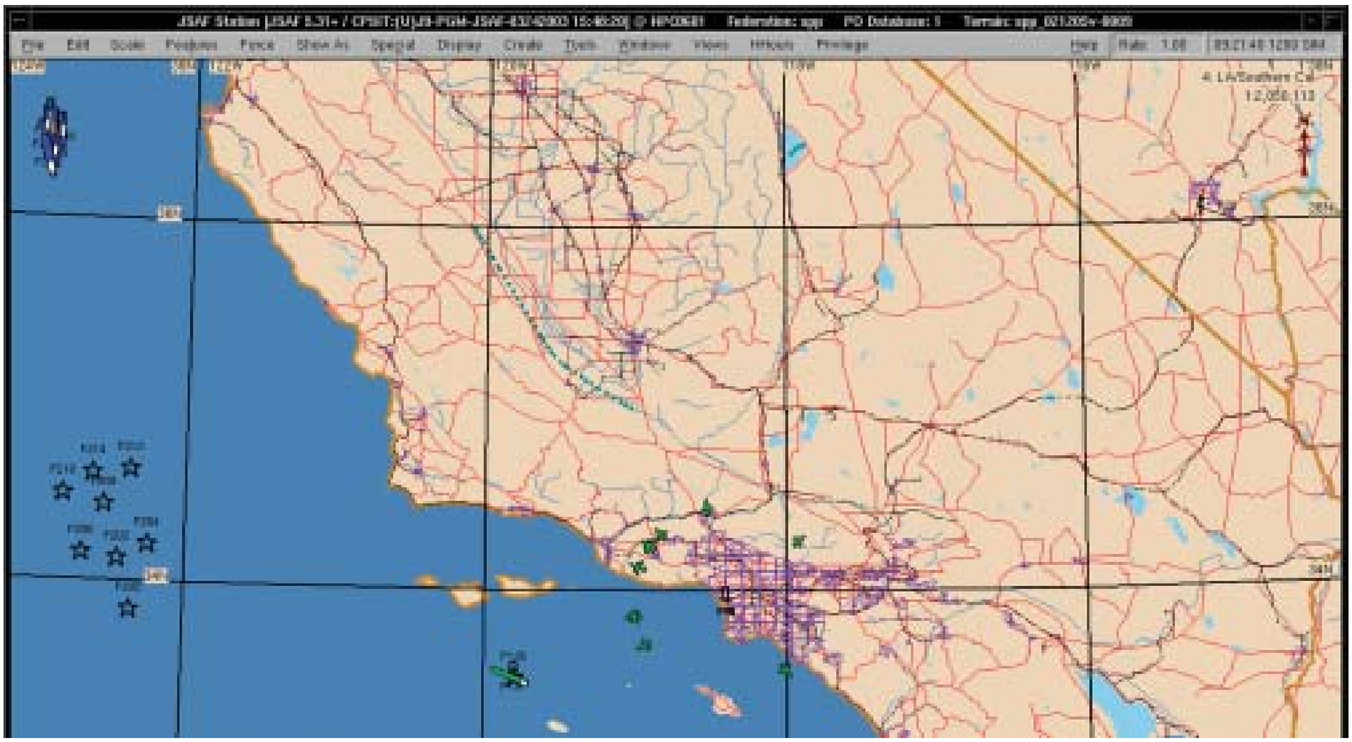


Figure 2. JSAF PVD

Figure 3. Stealth 3-D View of Battlefield

JESPP III was the next logical step in developing infrastructure for the Distributed Continuous Experimentation Environment (DCEE) that JFCOM’s web page describes as a capability “that will consist of modeling simulations, federations, software, and networks joined into one common computer infrastructure, which will feed training events and experimentations.”

Highlight

Users Reap Benefits of Recent System Upgrades

By Steve Wilson

In October 2002, the ASC MSRC conducted a major maintenance upgrade that promised to be far more challenging than any maintenance the ASC MSRC had previously attempted.

To meet this challenge, an Outage Team was formed months prior to the outage to identify, coordinate and manage the interdependencies of all planned activities. The Outage Team identified nine critical systems to upgrade and assigned separate teams to work each system in parallel. In preparation for the outage, the Team identified critical upgrades to be performed and the order in which they were to be performed. Dependent activities were identified, as well as a fallback position for every reasonable contingency.

In an effort to reduce the negative impact on the customer, system managers chose to implement the upgrades over an eight-day period. This decision was based on several factors:

- Every outage, regardless of duration, requires days of draining leading up to it. Draining results in lost cycles. Multiple outages instead of one would have resulted in multiple times the number of cycles lost in draining.
- Upgrades scheduled for the network, the High Availability File Server (HAFS), and the Mass Storage Archival Servers (MSAS) impacted all systems. A great deal of effort was made to make upgrades in parallel. Doing upgrades in a serial fashion would have extended the outage on single systems because of interdependences of the systems. For example, the MSAS upgrade alone took five days.
- The large number of upgrades increased the possibility of fall out. Maintenance week activities included periodic correction of problems, enabling us to quickly return to full production following the outage.

To mitigate risks, the team performed extensive testing on the Test And Development Environment (TADE), a separate parallel network equipped with small test boxes that mirror, on a much smaller scale, virtually all high performance systems on the production floor. Careful early planning and intense testing paid huge dividends as problems encountered in the TADE were corrected before upgrades were made on the production systems.

New equipment, new capabilities, and new IP addresses were all implemented during this maintenance period. The MSRC network staff replaced the existing border router with a Juniper Networks M20 router, which is capable of supporting multiple Gigabit Ethernet, OC-12 Asynchronous Transfer Mode (ATM), and OC-12 Packet Over SONET (POS) interfaces. (It even supports OC-48 POS interfaces.) The Juniper M20 provides the MSRC a significant increase in routing capability, and prepared the MSRC for the DREN upgrade to Gigabit Ethernet. The network staff also upgraded the Gigabit Ethernet network by enhancing the Foundry Networks BigIron 15000 switch-routers to support 9000-byte "jumbo frames," resulting in a much more efficient transfer of data between the compute and file servers. Not to be left behind, the ATM LANE network also received a router upgrade. A Cisco 7513, with two OC-12 ATM interfaces, was deployed to enhance the throughput on this network.

In addition to the network equipment upgrades, every IP address on every MSRC system was changed. This effort required months of planning and careful implementation. To accomplish this, dual Gigabit Ethernet networks, dual ATM networks, and dual Ethernet/Fast Ethernet networks were deployed, one on each IP address space. The system administrators were then able to move their systems from one network to the other while minimizing the loss of connectivity. Once the entire center had completed the IP address transition, the networks supporting the old address space were decommissioned.

The Sierra Cluster 2.5 (kite) operating system upgrade on the Compaq SC-40/45 systems was identified as a particularly risky activity. To reduce the risk, the Compaq SC-40 was brought down a week prior to the scheduled outage and made available for testing. Although the SC-40 was, as a consequence, down an extended period of time, user impact was small due to the fact that the users still had 209 of the 225 nodes of the consolidated SC-40/45 system available for processing. Due to the lessons learned with the SC-40, the upgrades on the SC-45 proceeded without problems.

The method used to upgrade the redundant Key Distribution Centers (KDCs) and User Authentication Servers (UASs) resulted in virtually no user downtime for these systems. Specifically, KDC2 and UAS2 were pre-staged one week prior to the outage. Upgrades were completed on these systems, which were placed in operation when KDC1 and UAS1 were brought down for upgrade one week later.

Also included in the maintenance outage was a major upgrade of the MSAS. Upgrades included moving to the Solaris 2.8 Operating System, adding two 400 MHZ CPUs making a six CPU machine, increasing disk cache capacity to 4 TB or 800 GB/file server, installing new drives, and performing silo maintenance.

As a result of extensive and intricate planning, fully operational and upgraded systems were placed back into production as scheduled for the user community. Despite all the activities and significant risks of this very ambitious upgrade to the entire environment, all system upgrades were hugely successful. Success can be attributed, in large part, to the hard work, professionalism, and attention to detail of a highly skilled MSRC staff. Members of the Outage Team were: Darwin Adams, Frank Barnhart, Win Bernhard, Tony DelSorbo, Mark Dotson, Jay Grover, Larry Haas, Mahmoud Hanafi, Tammy Hanafi, Frank Hughes, Hank Laughlin, Gary Meyer, Vaughn Noga, Nick Pellegrini, Mark Poe, Pete Sampson, Mark Schultz, John Sprinkle, Ann Ware, Tracey Wilson, Tim Yeager, CSC; Joe Robichaux and Don Cable, IBM; Bill Aders, SGI; Gary Floyd, Compaq; Rich Gestrich, Bill Johnson, Gary Louden, Carl Radeloff, Gary Sivak, Ron Trimble, ASC/HPTS; Ralph McEldowney and Dave Potts, ASC/HPTI.

Upcoming Conferences

June 11 - 13, 2003
SOFTVIS 2003
International Symposium of Software Visualization
San Diego, California

July 6 - 9, 2003
ICME 2003
IEEE International Conference on Multimedia & Expo
Baltimore, Maryland

July 17 - 20, 2003
Dayton Air Show
Dayton International Airport
Dayton, Ohio

July 20 - 24, 2003
2003 Summer Computer Simulation Conference (SCSC'03)
Montreal, Canada

July 27 - August 1, 2003
SIGGRAPH 2003
San Diego, California

September 27 - October 1, 2003
PACT 2003
12th International Conference on Parallel Architectures and Compilation Techniques
New Orleans, Louisiana

October 19 - 24, 2003
Vis 2003
Seattle, Washington

October 20 - 21, 2003
IEEE Symposium on Parallel and Large-Data Visualization and Graphics
Seattle, Washington

October 21 - 23, 2003
InfoTech 2003
Dayton, Ohio

November 15 - 21, 2003
Supercomputing Conference 2003
Phoenix, Arizona

Adsorbate Effects of Oxygen Atoms on the Field Emission of Single-wall Carbon Nanotubes

Researchers

Xiaofeng Duan
Major Shared Resource Center for High Performance Computing, ASC/HPT

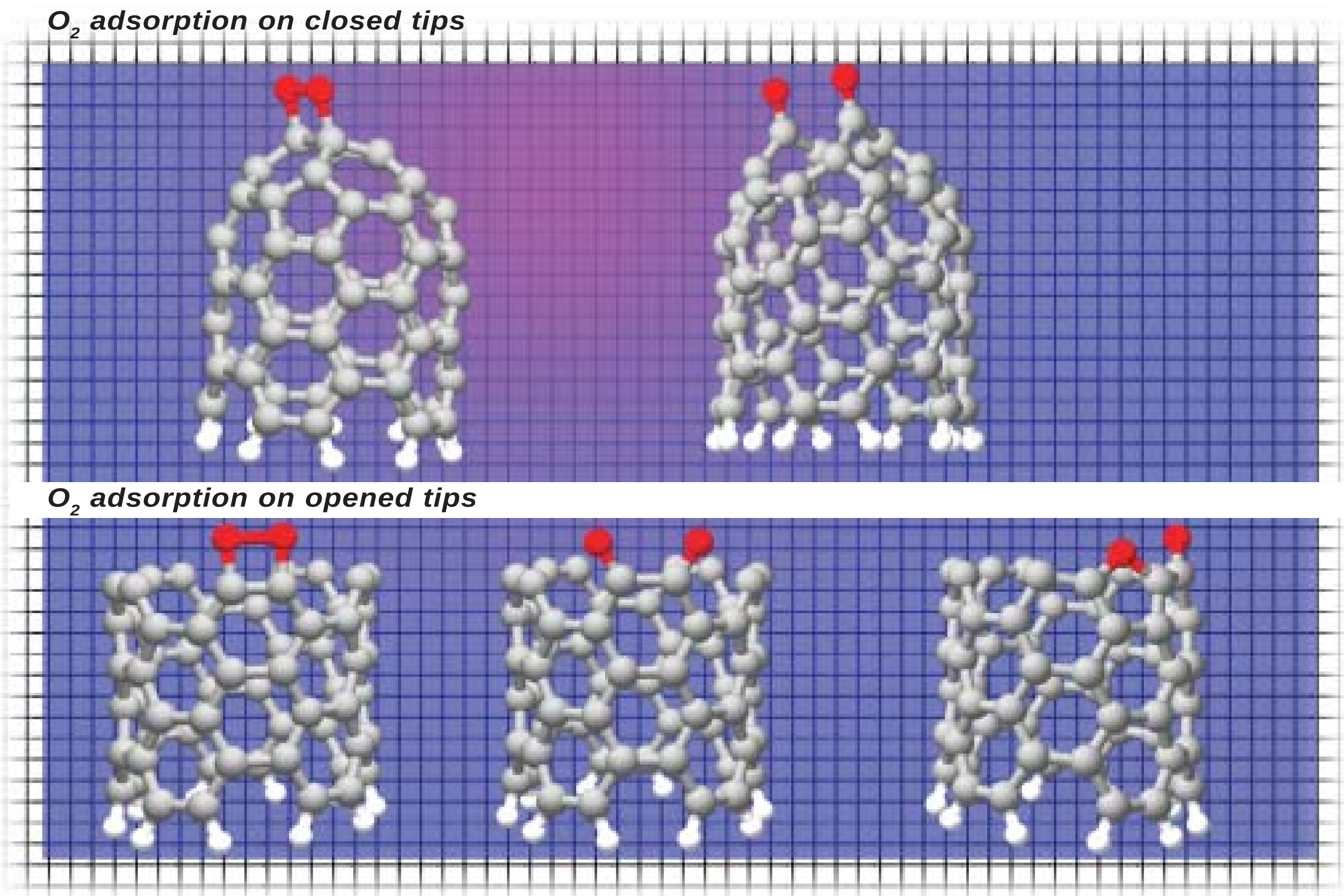
Brahim Akdim and Ruth Pachter
Air Force Research Laboratory, Materials & Manufacturing Directorate, AFRL/ML

Recently, carbon nanotubes attracted considerable attention in field emission applications, due to their capability of emitting high currents (up to 1 A/cm^2) at low field (~ 5 V/μm)[1]. Indeed, advances in the production of well-aligned carbon nanotubes, and control over their deposition, made it possible to use carbon nanotubes (CNTs) as potential emitters[2]; a prototype of a flat panel with color display[3] has already been achieved. Notwithstanding the rapid technological progress, there are still unanswered questions in terms of the emission mechanisms of CNTs.

The field emission properties have previously been explained in terms of Fowler-Nordheim's (FN) theory[4], which suggests that the emission occurs through a tunneling process. However, recent experiments[5] show a deviation of the current-voltage (I-V) characteristics from the FN model. Saito et al.[6] suggested that the deviation is due to the nonmetallic local density of states present at the tips, while Bonard et al.[7] reported that this deviation results from the interaction between tubes; other reports suggest that the deviation occurs due to gas adsorption at various CNTs sites[8]. Although studies of the effects of gas adsorption on CNTs, and in particular of O_2, have been previously reported experimentally[9], and theoretically[10,11,12,13,14], insight into the detailed chemistry at the adsorption sites under an external field has not been adequately explored yet. In this work, we focused on O_2 adsorption on single-wall CNTs, with the aim of gaining an understanding of the adsorption mechanisms at various sites for different tube geometries, and explain the effects on the emission current behavior. Density functional theory (DFT) calculations were carried out on HPC machines at the ASC MSRC, using an all-electron linear combination of atomic orbitals (LCAO), with the pbe functional and double numerical polarized (DNP) basis sets (using Accelrys DMol3[15] package).

We investigated the mechanisms of O_2 adsorption on closed and open tips of C (5,5) nanotubes as shown in the figures below. The results show that O_2 chemisorption is an endothermic reaction on a capped tip, with the (h-p) site being energetically more favorable than the (h-h) site. However, if the thermodynamic conditions exist for a chemisorption to occur, an energy barrier larger than 3.0 eV is required to etch the tube. In the open-ended tip, all the interactions we examined were exothermic with lower adsorption energies. This suggests that the current suppression observed experimentally when a CNTs sample was exposed to O_2, is due primarily to the presence of a high percentage of open-ended tips or tubes with structural defects.

Calculations of the effects of an applied field show that an applied voltage lowers the adsorption energy of closed tips of nanotubes, thus setting the conditions for a chemisorption process to take place, which then, in turn, leads to etching. A 2 eV/Å increase in the field strength alters significantly the structural parameters, resulting in a lower energy barrier for an etching process to occur. As for the open tips, no desorption mechanism is initiated at a field strength of 1 eV/Å. A higher field strength of 2 eV/Å was also tested for oxygen atoms desorption, and although longer O-C bonds were observed, bonds breaking did not occur at this field strength. The emission current is well known to depend strongly on the work function, approximated in our study by the first ionization potential (IP). Our calculations indicate that under a zero electric field, a moderate increase in the IP of about 2% was observed upon O_2 adsorption. This implies that O_2 adsorption does, indeed, play a role in the current suppression observed experimentally[16].



O_2 adsorption at closed and open tips of single wall nanotubes.

References

[1] J.-M Bonard, M. Croci, C. Klinke, R. Kurt, O. Noury, and N. Weiss, Carbon 40, 1715-1728 (2002).

[2] W. A. Deheer, A. Chatelain, D. Ugarte, Science 270, 5239 (1995).

[3] W. B. Choi, D. S. Chung, J. H. Kang, H. Y. Kim, Y. W. Jin, I. T. Han, Y. H. Lee, J. E. Jung, N. S. Lee, G. S. Park, and J.M. Kim, Apply. Phys. Lett 75, 3129-3131 (1999).

[4] R. H. Fowler and L. Nordheim, Proc. R. Soc. London, Ser. A 119, 173 (1928).

[5] R. Collazo, R. Schlesser, and Z. Sitar, Diamond and Related Mater. 11, 769-773 (2002).

[6] Y. Saito, K. Hamaguchi, T. Nishino, K. Hata, K. Tohji, A. Kasuya, and Y. Nishina, Jnp , J. Apply. Phys. Part 2 L1340, 36 (1997).

[7] J.-M. Bonard, J.-P. Salvetat, T. Stockli, W. A. De Heer, L.Forro, and A. Chatelain, Apply. Phys. Lett. 73, 918 (1998).

[8] S. C. Lim, Y. C. Choi, H. J. Jeong, Y. M. Shin, K. H. An, D. J. Bae, Y. H. Lee, N. S. Lee, and J. M. Kim, Adv. Mater. 13, 563 (2001).

[9] H. Ulbricht, G. Moos, and T. Hertel, Phys. Rev. B 66, 075404 (2002).

[10] C.-Y. Moon, Y.-S Kim, E.-C. Lee, Y.-G Jin, and K. J. Chang, Phys. Rev. B 65, 155401 (2002).

[11] X.Y. Zhu, S. M. Lee, Y. H. Lee, and T. Frauenheim, Phys. Rev. Lett. 85, 2757 (2000).

[12] J. A. Steckel, K. D. Jordan, and P. Avouris, J. Phys. Chemi. A 106, 2572 (2002).

[13] N. Park, S. Han, and J. Ihm, Phys. Rev. B 64, 125401 (2001).

[14] S.-H. Jhi, S. G. Louie, and M. L. Cohen, Phys. Rev. Lett. 85, 1710 (2000).

[15] Dmol3, Accelrys, Inc.

[16] S. C. Lim, Y. C. Choi, H. J. Jeong, Y. M. Shin, K. H. An, D. J. Bae, Y. H. Lee, N. S. Lee, and J. M. Kim, Adv. Mater. 13, 563 (2001).

Service Center Provides Top-Notch Customer Service

By Ann Ware

The ASC MSRC Service Center, a branch of the Customer Assistance Center (CAC), is always available to serve our user community. The Service Center is responsible for the first tier of support to the HPC customer. The center handles the full spectrum of questions, from initial questions to those of the most sophisticated supercomputer users. The Service Center staff is available to assist users with application development, modification, and execution offering "live" support 7am to 5pm EST, Monday through Friday. After hours support provided by the Operations Support staff includes phone support, service requests logging, and delivering initial service request responses and current system status information to customers. This gives customers the ability to reach personnel to check on system status, network problems and job losses during evenings and long holiday weekends. If the Operations staff is not immediately available to take calls due to job priorities, such as system failures, user calls are dispatched to the voicemail system. In such cases, customers will receive a response from the first available resource. Established procedures are in place to ensure our customers receive the highest quality customer support. Those procedures are explained below.

After the problem is reported, the ASC MSRC Service Center performs the following:

1. Capture details from the customer concerning user information, hardware/software involved, and as much as can be determined regarding the problem.
2. Create a Service Ticket using the Systems Management And Reporting Tool (SMART) Service Request Subsystem (SRS) application.
3. Use expertise, HPC access, and SMART SRS search capabilities of past Service Tickets to determine whether the problem is one that can be resolved immediately.
    a) If so, the Service Center representative will give the customer an immediate answer. Fulfilling the role of 1st tier support, the Service Center representative is recorded as the Technician that resolved the request. The Service Ticket status will be entered as "Resolved".
    b) If the problem cannot be resolved immediately, the Service Center representative will assign the appropriate 2nd tier technical support team. The Service Ticket status will be entered as "Open". A single member of the 2nd tier support team takes ownership of the Service Ticket with the approval of the support team or manager.

Once the Service Ticket is created, a member of the assigned technical support team will process according to the following:

a) Evaluate and discuss the problem with other technical support personnel.
b) Attempt to reproduce the problem.
c) Request additional information from the user regarding the problem.

The Technician either contacts the user directly or replies to the email generated by the automated Service Ticket tracking system. The Service Center monitors all Service Ticket responses and, upon request, contacts the user for the detail requested by the Technician.

The Service Ticket originator is sent an email message containing details of a Service Ticket status change in the following cases:

Initial request → Open
Resolved → Open

An email is sent to the service request originator upon opening a Service Ticket with the Service Center or when a formerly resolved ticket is reopened due to a repeat of the initial problem or dissatisfaction with the proposed resolution.

Open → Resolved

After a resolution is offered, a summary of the solution is sent via email.

Open → On Hold

When a resolution is delayed unexpectedly, perhaps due to a request for information from a 3rd party, the Originator is notified via email and given an estimated resolution timeframe.

A Service Ticket is escalated to management's attention according to defined priority levels (PL) and severity levels (SL) as follows:

Priority Level Definitions

- Priority 1: Multiple users affected.
- Priority 2: Single user or Project affected.
- Priority 3: Issue that has a temporary "workaround" solution.

Severity Level Definitions and Examples

- Severity 1: Critical, Major System Element Down - any HPC outage, hub/switch, router failure, MSAS, Network Anomalies
- Severity 2: Urgent - Application or Infrastructure related problems
- Severity 3: Important - Single User problems

Although subject to change, the table below represents the valid PL/SL combinations for Open service requests. Also noted is the corresponding number of *business* days (Monday-Friday) that must pass without activity on a particular service request prior to escalation:

		Severity Level					
		SL 1		SL 2		SL 3	
Priority Level	PL 1	2	4	3	6		
	PL 2			4	8	5	10
	PL 3					6	12
		Esc 1	Esc 2	Esc 1	Esc 2	Esc 1	Esc 2

An Escalation 1 (Esc 1) notification will be sent to the Group/Tech and associated Manager. An Escalation 2 (Esc 2) notification will be sent to the Group/Tech, associated Manager, and Program Manager and Deputy Program Manager.

The ASC MSRC Service Center is committed to providing top-notch customer service to our users and welcomes your comments. Contact the Service Center via email at *msrchelp@asc.hpc.mil* or by dialing toll-free, 1-888-677-2272.

Making the ASC MSRC HPC Environment Easier to Use

By Daniel Schornak

The ASC MSRC high performance computing environment has undergone an evolution over the years as it has brought expanded computational capability to the DoD researcher. This evolution is not without some challenge for the user community as it performs code migration, or porting, to a new computing platform. Compound this effort with the fact that other MSRCs are also evolving, the user could be overwhelmed in learning the changes occurring within each of the sites' computing environments. The introduction of a new platform could require the introduction of a new scheduling system that the user has not experienced. The ASC MSRC has incorporated measures that may better assist utilizing the ASC MSRC computing environment.

The Practical Supercomputing Toolkit – (www.pstoolkit.org) The ASC MSRC, as is true of the other MSRC sites, has incorporated components associated with the Practical Supercomputing Toolkit, also known as the Uniform Command-Line Interface (UCLI). Incorporation of this toolkit provides a uniform manner in which to move data between high performance computing systems and the mass storage unit (command: **archive**).

To provide a transparent means of generating a platform-specific batch script file, the user simply creates a "generic" batch script file and executes the UCLI tool command "qprep" on that script.

archive(1) PSTOOLKIT archive(1)

NAME

archive - perform basic file-handling operations on the local archival storage system.

SYNOPSIS

archive put [putopts] file1 [file2 ...]
archive get [getopts] file1 [file2 ...]
archive mv* [mvopts] file1 [file2 ...] target
archive rm* [rmopts] file1 [file2 ...] archive ls [lsopts] [file1 ...]
archive stat [statopts] [*name*]
archive mkdir [mkdiropts] dir1 [dir2 ...]
archive rmdir* [rmdiropts] dir1 [dir2 ...]
archive chmod* [chmodopts] *mode* file1 [file2 ...]
archive chgrp* [chgrpopts] group file1 [file2 ...]
archive chown* [chownopts] owner[:group] [file1 ...]

DESCRIPTION

archive provides users with a uniform, site-independent command interface to the local archival storage system, eliminating the need to learn the myriad syntactical variations that appear at different institutions to perform essentially identical archival file management tasks.

COMMANDS

Each instance of **archive** performs the file-management command identified by **archive**'s first argument: put, get, mv*, rm*, ls, stat, mkdir, rmdir*, chmod*, chgrp*, or chown*. Each command accepts a set of arguments as well as a set of command-line options described in the OPTIONS section below. If multiple archival storage facilities are available at a particular site, all of the commands act on the default system only, unless another system is specified with the -asf *host* option.

* The current version of **archive** does not support the commands indicated with asterisks (*). Later versions will incorporate these additional commands.

qprep(1) PSTOOLKIT qprep(1)

NAME

qprep - Translate job-submission scripts from a platform independent format to the local, platform-dependent format.

SYNOPSIS

qprep [key1=value1[key2=value2 ...]] filename

DESCRIPTION

qprep provides users with a uniform, site-independent command interface to the local queuing system, eliminating the need to learn the myriad syntactical variations that appear at different institutions to perform essentially identical job-submission tasks.

qprep translates a script from a site-independent format (described below) into a site-dependent format, typically one using NQS (Network Queuing System), PBS (Portable Batch System), or a similar queuing system. The translated script is written to a new file, and may optionally be submitted to a queue. Scripts written to the **qprep** standard will be usable at any site where **qprep** is implemented, regardless of the target queuing system.

DIRECTIVE SYNTAX

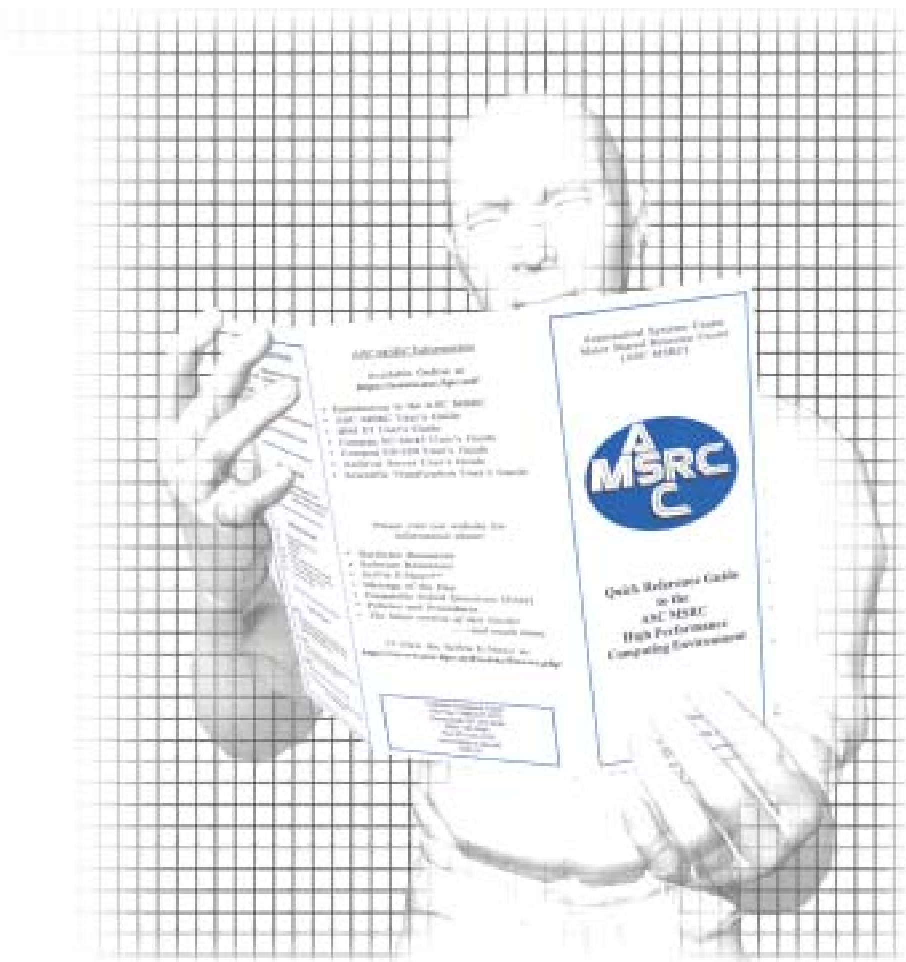
Options to **qprep** are given in the form of key-value pairs, called "directives". These may be given either at the command line, separated by white space, or in the preamble to a job script.

The file is created for the platform on which “qprep” is executed. (command: **qprep**).

At the ASC MSRC, qprep will generate the platform-specific script for Portable Batch Service (PBS), LoadLeveler, or Load Sharing Facility (LSF). Help files associated with both commands are available within the ASC MSRC environment (man archive; man qprep).

Quick Reference Guide to the ASC MSRC High Performance Computing Environment

Having the right command at your fingertips is the goal of this Quick Reference Guide. The guide answers questions such as what compilers, debuggers, and editors are available on the various HPC systems, as well as good-to-know batch system commands to check or modify the status of your queued or running job. Environment variables, some Unix commands, available documentation, and where to get assistance with additional questions are also covered. This guide is available directly from the ASC MSRC web site as a PDF file for easy printing, or by request through the ASC MSRC Customer Assistance Center *(msrchelp@asc.hpc.mil)*. This is a “got to have” guide.



Tecplot

By Darwin Adams

The Scientific Visualization (SciVis) Laboratory recently hosted a Vendor Day event featuring Tecplot 9.2, and the add-on package Computational Fluid Dynamics (CFD) Analyzer 3.0. More than twenty researchers from the Air Force Research Laboratories' Propulsion, Air Vehicles, and Sensors Directorates, met with representatives from Amtec Engineering. The event provided the opportunity for Tecplot users, novice and experienced, to get a first-hand overview of the new features available in Tecplot 9.2 and the opportunity to see the newest add-on to Tecplot, CFD 3.0.

The open format of this Vendor Day event provided an informal setting where the software developers could exchange problem-solving information directly with the researcher. Tecplot representatives presented future expectations of Tecplot in the research area. Current users were assured that Tecplot will continue to be expanded upon and developed in the future. The event featured a live demonstration using the CFD Analyzer add-on to analyze CFD data. Tecplot CFD Analyzer saves time finding, extracting and processing the critical information. CFD Analyzer provides many of the functions commonly used to calculate variables and perform integrations.

Through this event, the ASC MSRC SciVis Laboratory has empowered both research and software communities to focus on identifying pre- and post-processing and visualization solutions to better enable research activities. The researcher has an opportunity to address concerns and resolve complex visualization problems. The software vendor has an opportunity to instruct and inform attendees of software enhancements, techniques, and new products.

An alternative resource for information about Tecplot is the "*Contours E-Newsletter*", freely available from Amtec Engineering. *http://www.amtec.com/contours/index.html.*

Additional events will be scheduled throughout the year. A request for additional information should be emailed to *msrcenws@asc.hpc.mil*.

IE Update

By Jeff Graham

A new tool for the Service Agency Approval Authorities (S/AAAs), Site Account Managers (SAMs), users, and managers within the HPCMP is finally here. After a long and arduous journey, the Information Environment (IE) is alive and kicking on servers at the ASC MSRC, with about 25 individuals logging in and using the tools every day. Although several minor problems are still causing some consternation, the automated file transfers are working well and the IE tool has been very stable. ASC MSRC Service Desk and database personnel continue to do a super job of keeping IE up and running as well as facilitating the solutions to varying user concerns and problems.

A significant training event occurred in early March 2003 when most S/AAAs received IE training during their annual meeting. Although one of the winter's many snowstorms impacted the length of the session, a large segment of the folks who will benefit the most from IE were in attendance. Ms. Jeanie Osburn, Training Lead from the IE Integrated Product Team (IPT) provided the training. Additional training events are being planned.

In order to ensure that IE will fulfill the requirements of our community and overcome identified bugs in version 1.0, the IE IPT has leveraged all available avenues to collect and prioritize bugs and potential enhancements. The first set, containing the most critical bugfixes and enhancements, were addressed and corrected in version 1.1. A following set of bugfixes and enhancements will be implemented in version 1.2, scheduled for release in late June. This means that the most critical improvements needed by IE users will be available before the crunch time leading up to account renewals and allocations for FY04.

Another significant event is currently underway and should be nearly complete when this journal is published. The host site responsibility currently provided by ASC will be transitioned to the Information Technology Laboratory (ITL) at ERDC. This means that after the planned June transition, ITL personnel will be responsible for running IE and servicing questions and concerns. The HPTi developers will remain on contract until the end of FY03 to provide consultation and development activities. After 1 October 2003, ITL personnel will handle all support and development activities associated with IE. IE users should see minimal impact during the transition. In addition to the transition from ASC to ITL, the IE IPT is working on the details for the deployment of a backup capability to be provided at NRL-DC. This will ensure the tool will be available at all times for users.

Plans for IE revolve around a goal of having a robust and reliable tool available and in place at ITL in order to smoothly handle all FY04 account and allocation activity. ASC MSRC support staff, HPTi's developers, ITL contractors, IE IPT members, and HPCMPO personnel (Larry Davis and Cathy McDonald) have worked hard to realize that goal.

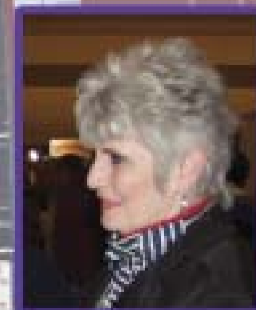
CSC Wins Support Contract

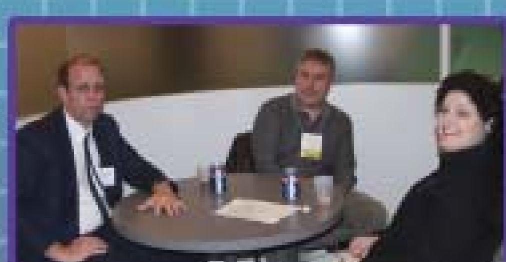
By Donna G. Klecka
CSC Program Manager

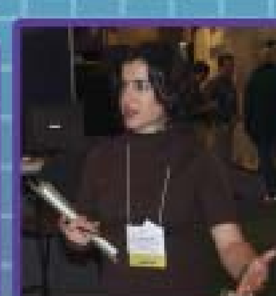
On behalf of our team, I am thrilled that CSC has been selected to provide operations and user support at the ASC MSRC under a new GSA Task Order. Over the past six years, CSC has had the privilege of working as a team with government personnel and the user community. Together we have experienced great success in providing premier HPC capabilities, which empower our customers to provide support to the warfighter. The ASC MSRC has consistently delivered compute systems, which meet or exceed user requirements. We were one of the first to establish a highly available mass storage system, which greatly improved file archival and retrieval times. One of our most recent successes is the implementation of the remote disaster recovery capability. This capability enhances the site's ability to protect user data as well as ensure continuity of service in the event of a local catastrophe. These successes along with many others are the result of the dedication and commitment of the ASC MSRC government and CSC staff working together to achieve our mission. I am proud of what we have achieved as a team, and I look forward to even greater accomplishments in the future.

SC2002

Baltimore, Maryland





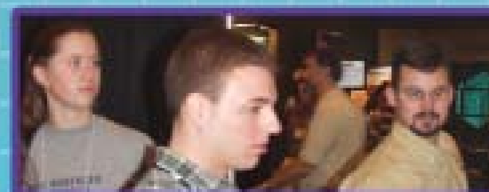










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